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Title:	On Two-Phase Pressure and Temperature Equilibration with Mie-Grüneisen Equations of State
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On Two-Phase Pressure and Temperature Equilibration with Mie-Grüneisen Equations of State (LA-UR-21-23970)

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In the course of reactive flow modeling, the phases of high explosive (HE) reactants and products introduce additional degrees of freedom to the underlying hydrodynamic equations of compressible reactive fluid mechanics. Hydrodynamic simulations track the bulk (mixture) conservation properties of mass, momentum and energy. When multiple phases are introduced, one must decide on appropriate closure rules to determine the relative phase volumes and energy distribution between the phases. One typical closure is to assume that the phases are in pressure and temperature equilibrium. Here, the requisite equations of p-T equilibration are explored for Mie-Grüneisen Equations of State (EOS). Examples with Davis reactants and Davis products EOSs will be given. The Davis forms are used in both the WSD [1] and AWSD [2] reactive flow models.

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I.   GOVERNING EQUATIONS

From hydrodynamic equations of two phase reacting flow, one has the conservation laws of mass, momentum and energy, in addition to a rate law representing the conversion of reactants to products:

$$\frac{D\rho}{Dt} + \rho\vec{\nabla} \cdot \vec{u} = 0 \tag{1}$$

$$\rho\frac{D\vec{u}}{Dt} + \vec{\nabla}p = 0 \tag{2}$$

$$\frac{De}{Dt} + p\frac{D(1/\rho)}{Dt} = 0 \tag{3}$$

$$\frac{D\lambda}{Dt} = r \tag{4}$$

where ρ is the mixture density, $\vec{u}$ is particle velocity, p is pressure, e is mixture specific internal energy, λ is the mass fraction of products and r is the rate of production of products from reactants. For standard single phase flow, the last equation is absent, and one only needs an incomplete EOS, $p(\rho, e)$, to close the mass, momentum and energy equations. Temperature, in particular, is not required.

For reactive flow, where there exists separate reactants and products EOSs, one needs additional rules to close the system of equations. One such common rule is to assume that each phase (reactant and product) is in pressure and temperature equilibration. These two statements then dictate how the energy and volume fractions are partitioned. Prior to getting into the details, it is worthwhile to define some notation. In particular, items with the subscript r will denote reactants and subscript p will denote products. So, we have:

$$\rho_r = \text{density of reactants}$$

$$\rho_p = \text{density of products}$$

$$e_r = \text{specific energy of reactants}$$

$$e_p = \text{specific energy of products}$$

$$v_r = \frac{1}{\rho_r} = \text{specific volume of reactants}$$

$$v_p = \frac{1}{\rho_p} = \text{specific volume of products}$$

It is also useful to define the volume fractions of the reactants and products. The symbol ϕ is often used for volume fraction (see for example [3, 4]). This is not to be confused with Φ used by Stewart, et al [5] to define the ratio of specific volumes $\Phi = v_r/v_p$. The volume fraction of products is related to the mass fraction of products, λ, and mixture density, ρ, and products density, ρ_p, by:

$$\phi_p = \frac{\rho}{\rho_p}\lambda \tag{5}$$

and since the mass fraction of reactants is $(1 - \lambda)$, we have similarly for the volume fraction of the reactants:

$$\phi_r = \frac{\rho}{\rho_r}(1 - \lambda). \tag{6}$$

The mixture specific volume is given by:

$$v = (1 - \lambda)v_r + \lambda v_p \tag{7}$$

Or equivalently, with ρ_r and ρ_p substituted for v_r and v_p.

$$1/\rho = (1 - \lambda)/\rho_r + \lambda/\rho_p \tag{8}$$

and the mixture specific internal energy is given by:

$$e = (1 - \lambda)e_r + \lambda e_p \tag{9}$$

II. PRESSURE-TEMPERATURE EQUILIBRATION, GIVEN λ, ρ AND e

Presuming we have expressions for pressure and temperature for the reactants and products in terms of their respective densities and specific energies, the basic equations of pressure and temperature equilibration can be cast into a system of 4 equations and 4 unknowns, by finding the roots of the equations:

$$(1 - \lambda)/\rho_r + \lambda/\rho_p - 1/\rho = 0 \tag{10}$$

$$(1 - \lambda)e_r + \lambda e_p - e = 0 \tag{11}$$

$$p_r(\rho_r, e_r) - p_p(\rho_p, e_p) = 0 \tag{12}$$

$$T_r(\rho_r, e_r) - T_p(\rho_p, e_p) = 0 \tag{13}$$

Typically from hydrodynamics, one knows λ, ρ and e. The contrary case of knowing λ, ρ and p, which often appears in initial and boundary conditions, is covered separately in a later section. Given the above 4 equations, we need to solve for ρ_r, ρ_p, e_r and e_p. One could simply solve the above 4 equations directly, but there are several simplifications that can be made. The first thing to note is that density of one constituent can be written in terms of the other constituent density, the mixture density, ρ, and mass fraction, λ. Likewise the energy of one constituent can be written in terms of the other constituent energy, the mixture energy, e, and mass fraction λ. This is generally true, even for arbitrary EOSs that are not of the Mie-Grüneisen form. But, with both EOSs of the Mie-Grüneisen form, one additional simplification can be made. Recall that for a Mie-Grüneisen EOS, one has a linear relationship between e and p. So, the energy distribution between the 2 phases can be solved explicitly, and the above 4 equations can be boiled down to a single equation in temperature equilibration. These ideas are explored in detail next.

First, it is worth while to write everything in terms of ϕ_p. The reason being is that the limits of ϕ_p are known to be the same as the limits of λ when $\lambda = 0$ and $\lambda = 1$. Future work may use these limits in an asymptotic fashion, such that accurate analytic limits may be employed in the limit of a single phase. And, like λ, ϕ_p is a well defined and continuous function for most flows. From equation 5, the density of the products is given as:

$$\rho_p = \frac{\rho}{\phi_p}\lambda \tag{14}$$

Likewise, given that $\phi_p + \phi_r = 1$, we can determine the density of the reactants as:

$$\rho_r = \frac{\rho}{1 - \phi_p}(1 - \lambda) \tag{15}$$

It is straightforward to show that equations (14) and (15) automatically satisfies the mixture specific volume relation, equation (10).

From equation (11), the specific energy of the reactants, e_r, can be solved for in terms of the mixture energy, e, mass fraction, λ, and e_p as:

$$e_r = \frac{e - \lambda e_p}{(1 - \lambda)} \tag{16}$$

For general EOSs, the previous 3 equations can be substituted into the pressure and temperature equilibration equations (12) and (13) to obtain 2 equations for the 2 unknowns ϕ_p and e_p.

Prior to further simplifications, the Mie-Grüneisen forms for the reactants and products pressure are given by:

$$p_r(\rho_r, e_r) = p_r^s(\rho_r) + \rho_r \Gamma_r(\rho_r)(e_r - e_r^s(\rho_r)) \tag{17}$$

and

$$p_p(\rho_p, e_p) = p_p^s(\rho_p) + \rho_p \Gamma_p(\rho_p)(e_p - e_p^s(\rho_p)). \tag{18}$$

Here, the superscript s refers to the reference curve, in particular for the Davis EOS forms, the reference curves are isentropes. But, the following simplifications hold true for other reference curves as well. The simplification lies in the fact that the specific energy appears linearly in the Mie-Grüneisen EOS. The pressure equilibration, equation (12), for the above Davis EOS forms, becomes

$$p_r^s(\rho_r) + \rho_r \Gamma_r(\rho_r)(e_r - e_r^s(\rho_r)) - p_p^s(\rho_p) - \rho_p \Gamma_p(\rho_p)(e_p - e_p^s(\rho_p)) = 0 \tag{19}$$

One can explicitly substitute equation (16) into this equation and solve for e_p:

$$e_p = \frac{p_r^s(\rho_r)(1 - \lambda) + \rho_r \Gamma_r(\rho_r)(e - e_r^s(\rho_r)(1 - \lambda)) - \left(p_p^s(\rho_p) - \rho_p \Gamma_p(\rho_p)e_p^s(\rho_p)\right)(1 - \lambda)}{\rho_r \Gamma_r(\rho_r)\lambda + \rho_p \Gamma_p(\rho_p)(1 - \lambda)} \tag{20}$$

In the above, the ρ_r and ρ_p are themselves computed in terms of ρ, λ and ϕ_p, and thus e_p is written in terms of known quantities and ϕ_p. This can then be used to compute e_r from equation (16).

Now, these values can be substituted into the temperature equilibration equation (13), to form a single equation in terms of the unknown volume fraction ϕ_p. Namely, we seek the root of the equation:

$$F_p(\phi_p) = T_r(\rho_r(\rho, \lambda, \phi_p), e_r(e, \rho, \lambda, \phi_p)) - T_p(\rho_p(\rho, \lambda, \phi_p), e_p(e, \rho, \lambda, \phi_p)) = 0 \tag{21}$$

where, again, ρ, λ and e are all known, and the only unknown is ϕ_p. Here, the subscript p in F_p is to indicate that the pressure is unknown. In a subsequent section, a different F will be derived for when the pressure is specified.

III.   DAVIS REACTANTS AND PRODUCTS EQUATION OF STATES

A.   Davis Reactant Equation of State

The Davis reactants EoS form in terms of $p_r(\rho, e)$ [10] is expressed as:

$$p_r(\rho, T) = p_r^s(\rho) + \rho \Gamma_r[e - e_r^s(\rho)] \tag{22}$$

where, the reference isentrope, $p_r^s(\rho)$ is:

$$p_r^s(\rho) = \begin{cases} \hat{p}\left[\exp(4By) - 1\right], & \rho < \rho_0 \\ \\ \hat{p}\left[\sum_{j=1}^3 \frac{(4By)^j}{j!} + C\frac{(4By)^4}{4!} + \frac{y^2}{(1-y)^4}\right], & \rho \geq \rho_0 \end{cases} \tag{23}$$

where, $y = 1 - \rho_0/\rho$ and $\hat{p} = \rho_0 A^2/4B$. Here, A, B, C are material constants and ρ_0 is the reference density.

The energy on the reference isentrope can be obtained by integrating reference pressure along the isentrope, $p_r^s(\rho)$:

$$e_r^s(\rho) = \int_{\rho_0}^{\rho} \frac{p_r^s}{\bar{\rho}^2} d\bar{\rho} + E_0 \tag{24}$$

$$e_r^s(\rho) = \begin{cases} \frac{\hat{p}}{\rho_0}\left[\frac{\exp(4By)}{4B} - y - \frac{1}{4B}\right] + E_0, & \rho < \rho_0 \\ \\ \frac{\hat{p}}{\rho_0}\left[\sum_{j=2}^4 \frac{(4B)^{j-1}y^j}{j!} + C\frac{(4B)^4 y^5}{5!} + \frac{y^3}{3(1-y)^3}\right] + E_0, & \rho \geq \rho_0 \end{cases} \tag{25}$$

The Grüneisen parameter, $\Gamma_r(\rho)$ is taken to be:

$$\Gamma_r(\rho) = \begin{cases} \Gamma_r^0, & \rho < \rho_0 \\ \\ \Gamma_r^0 + Zy, & \rho \geq \rho_0 \end{cases} \tag{26}$$

where, the constant Z defines the change of $\Gamma_r(\rho)$ with respect to density.

The reactant temperature, $T_r(\rho, e)$ can be derived to be:

$$T_r(\rho, e) = T_r^s(\rho)\left[\frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)}\{e - e_r^s(\rho)\} + 1\right]^{\frac{1}{1+\alpha_{st}}} \tag{27}$$

where, the tempertaure on the reference isentrope, $T_r^s(\rho)$ is defined as:

$$T_r^s(\rho) = \begin{cases} T_0\left(\frac{\rho}{\rho_0}\right)^{\Gamma_r^0}, & \rho < \rho_0 \\ \\ T_0 \exp(-Zy)\left(\frac{\rho}{\rho_0}\right)^{\Gamma_r^0 + Z}, & \rho \geq \rho_0 \end{cases} \tag{28}$$

The reactant isochoric specific heat, C_{vr} is given by:

$$C_{vr}(\rho, T) = C_{vr}^0\left(\frac{T}{T_r^s(\rho)}\right)^{\alpha_{st}} \tag{29}$$

The values of Davis reactants EoS parameters for PBX 9501 are provided in Table 1.

Table 1. Davis reactants EoS parameters for PBX 9501 [6].

A	B	C	ρ_0	Γ_r^0	C_{vr}^0	α_{st}	T_0	E_0	Z
2.3 mm/μs	3.3	0.2	1.836 g/cc	0.838	0.001067 kJ/g K	0.3662	297 K	5.60208 kJ/g	0

B. Davis Product Equation of State

The Davis products EOS expressed in terms of $p_p(v, e)$ [1] as:

$$p_p(v, e) = p_p^s(v) + \frac{\Gamma_p(v)}{v}[e - e_p^s(v)] \tag{30}$$

The reference isentrope, $p_p^s(v)$ is:

$$p_p^s(v) = p_c \frac{[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}]^{a/n}}{(v/v_c)^{k+a}} \frac{k - 1 + F(v)}{k - 1 + a} \tag{31}$$

where,

$$F(v) = \frac{2a(v/v_c)^{-n}}{(v/v_c)^n + (v/v_c)^{-n}} \tag{32}$$

and the energy of the reference isentrope is obtained as:

$$e_p^s(v) = E_c \frac{\left[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}\right]^{a/n}}{(v/v_c)^{k-1+a}} \tag{33}$$

where,

$$E_c = \frac{p_c v_c}{k - 1 + a} \tag{34}$$

The Grüneisen parameter is chosen to be:

$$\Gamma_p(v) = k - 1 + (1 - b)F(v) \tag{35}$$

The products temperature, $T_p(v, e)$ is given as:

$$T_p(v, e) = T_p^s(v) + \frac{e - e_p^s(v)}{C_{vp}} \tag{36}$$

where, the temperature on the products reference isentrope is defined as:

$$T_p^s(v) = T_c \frac{[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}]^{(a/n)(1-b)}}{(v/v_c)^{k-1+a(1-b)}} \tag{37}$$

where,

$$T_c = \frac{2^{-ab/n}}{k - 1 + a} \frac{p_c v_c}{C_{vp}} \tag{38}$$

Here, p_c, n, a, k and b are material parameters and v_c is the reference specific volume. The values of these PBX 9501 products EOS parameters are provided in Table 2.

Table 2. Davis products EoS parameters for PBX 9501 [6].

a	k	v_c	p_c	n	b	C_{vp}
0.684311	1.62149	0.745829 cc/g	5.38897 GPa	1.58683	1.25	7.3e-04 kJ/g K

IV. OBSERVATIONS, COMMENTS AND AN EXAMPLE

The above arguments are all relatively straightforward to implement for general Mie-Grüneisen EOSs. Clearly the limit of ϕ_p going to either zero or one will lead to singularities unless simultaneously λ also goes to zero or one. But importantly, there are usually issues with the EOSs prior to getting to those limits. Namely, the temperature of one of the phases will become negative (products) or imaginary (reactants). To avoid imaginary temperatures, say in equation (37) of [1], they have replaced the variable specific heat model with a constant specific heat model when the bracketed term of equation (37) becomes negative. That alleviates the issue with imaginary temperatures, but leads to inconsistencies in the EOS (but in reality that's unavoidable). The thought is that for realistic values of ρ, e and λ, once the p-T equilibrium routine has finished solving the actual temperature will be positive. Again, this was added for robustness of p-T solution. If, after p-T equilibration occurs, and one finds a negative temperature, the internal energy is apparently too low for a realistic solution. This all assumes the EOSs are thermodynamically well behaved.

Let's now look at a specific example of Davis reactants and Davis products EOSs. In particular, the parameters in the recent 2019 APS-SCCM paper [6] for PBX 9501 will be examined. The particular state is about half way through the reaction zone for a near CJ detonation wave with $D = 8.812$ mm/μs. See Table 3 for the mixture state.

Table 3. Mixture density, mixture energy and mass fraction for the test case 1.

ρ	e	λ
2.98696 g/cc	11.3669 kJ/g	0.501249

This should be a "typical" case for reactive flow. See figure 1 for a plot of $F(\phi_p)$. The good news is the function $F(\phi_p)$ *appears to be* monotonic over the range $0 < \phi_p < 1$, with only a single root. The bad news is that the function is singular at the ends of the domain, as expected. A poor initial guess for ϕ_p will cause grief for a Newton-based method, and many other "high-order" methods, without a good starting value. Note that the function F has units of Kelvin. It is also the case that for the vast majority of the region in ϕ_p, at least one of the temperatures is negative.

It is worthwhile zooming in near the root of $F(\phi_p)$. See figure 2 for plots of the reactant and product temperatures and $F(\phi_p)$. Near the root of interest, $\phi_p \approx 0.529663$, the functions are all well behaved. One does observe a "glitch" in T_r (and thus F), near $\phi_p \approx 0.5548$. This is caused by the model specific heat for the reactants becoming imaginary at larger values of ϕ_p, which cause the bracketed term of equation (37) of [1] to become negative. In this section, we've simply adopted the same "fix" as the authors of [1], where a constant specific heat is used when the term inside the brackets becomes negative. This drastic change in specific heat model is the cause of the "glitch." One could build a different fix, which, at least, leads to a continuous $T_r(\rho, e)$ and thus $T_r(\phi_p)$. This may be particularly useful for mixtures at low temperatures, where such a discontinuous behavior may lead to multiple roots in $F(\phi_p)$. This is explored in the next section.

It is also worth noting that the range where the EOSs are well behaved (i.e. positive temperatures) is quite narrow, spanning only $0.5187 < \phi_p < 0.5548$. In this narrow range of ϕ_p, the function $F(\phi_p)$ is quite well behaved, and given a starting guess value in this region will likely lead to fast convergence for high order root finding methods.

The final p-T equilibrium state for this case is given in Table 4. Note the sound speed, c, is only an approximate value given by central differences (see later sections), and it appears the sound speed computations are ≈ 10 significant figures accurate, but still need to be cross-verified with other thermodynamic techniques for mixtures [4]. Recall the definition of (isentropic) sound speed [7] as a function of $p(\rho, e)$:

$$c^2 = \left(\frac{\partial p}{\partial \rho}\right)_e + \frac{p}{\rho^2}\left(\frac{\partial p}{\partial e}\right)_\rho \tag{39}$$
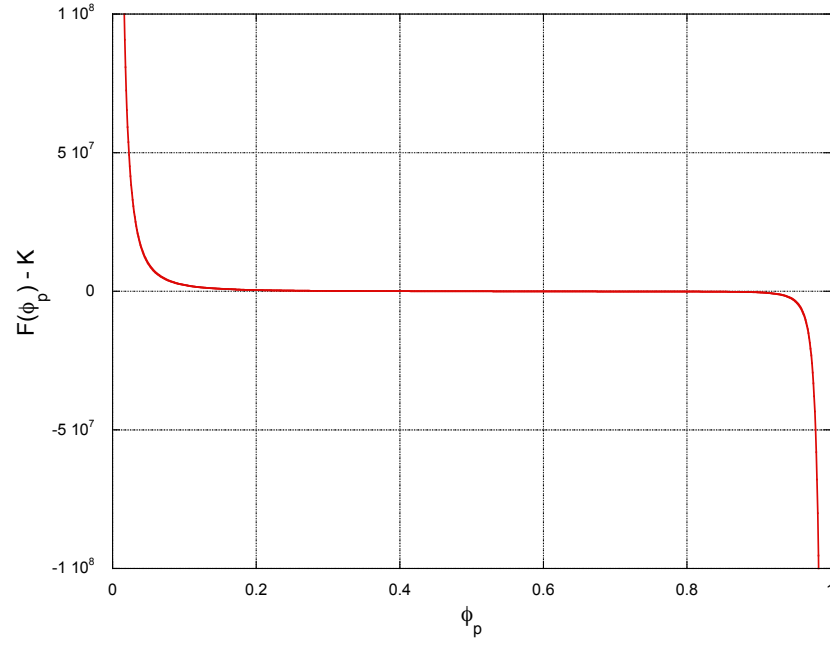
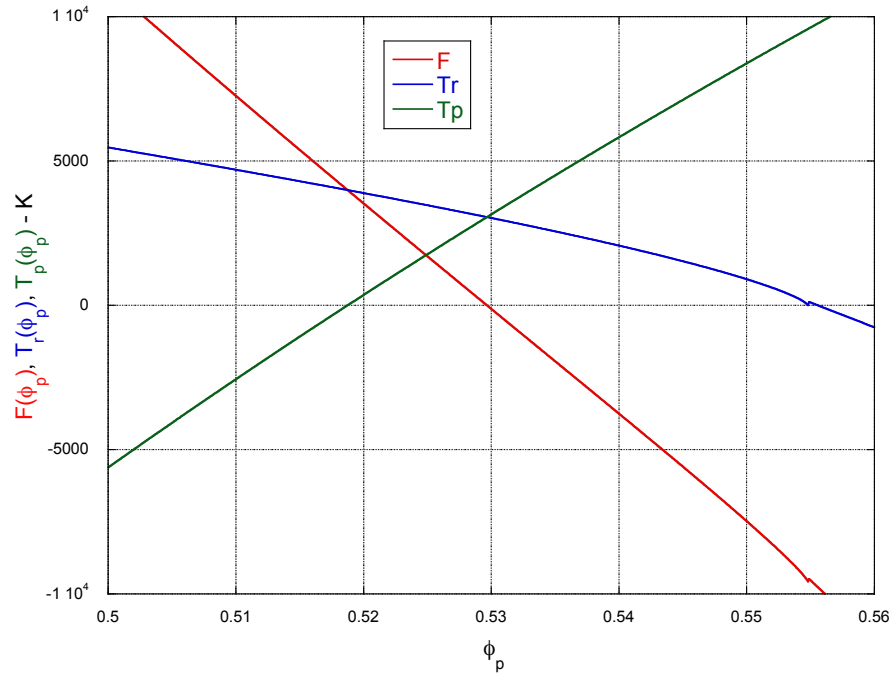FIG. 1. $F(\phi_p)$ over a wide range of ϕ_p for case 1.

FIG. 2. $F(\phi_p)$, $T_r(\phi_p)$ and $T_p(\phi_p)$ near p-T equilibrium root $\phi_p \approx 0.529663$.
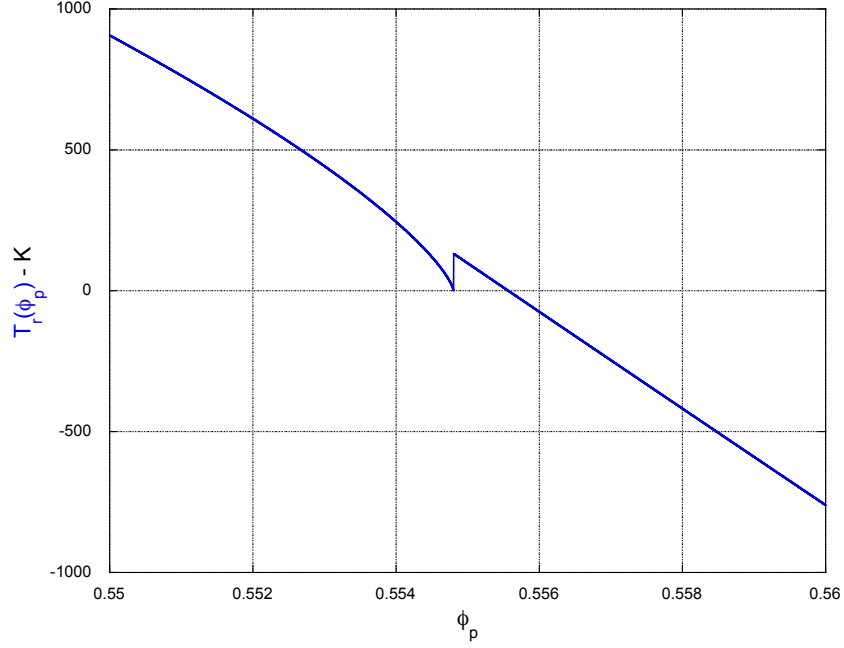
FIG. 3. $T_r(\phi_p)$ in the vicinity of where the model switches from a variable specific heat to a constant specific heat model to avoid imaginary temperature values.

Table 4. p-T equilibrium for the test case 1. Here, the sound speed, c, is computed with central differences.

ϕ_p	0.529663041576612
ρ_r	3.16740851485236 g/cc
ρ_p	2.82672302108026 g/cc
e_r	12.8258531224964 kJ/g
e_p	9.91521764492660 kJ/g
$p = p_r = p_p$	54.9354202145965 GPa
$T = T_r = T_p$	3056.64824932359 K
c	7.66180 km/s

Based on the final p-T equilibrium state, the thermodynamic properties of the reaction mixture can be calculated using the expressions provided in [4]. Table 5 summarizes the thermodynamic properties of the reactants, products and mixture. The thermodynamic expressions for the mixture properties are presented in the Appendix section. It is expected that the sound speed, as computed with the thermodynamic relations, will be more accurate than the central difference approximation. For this particular case, they agree to 6 significant figures.

Table 5. Thermodynamic properties of reactants, products and equilibrium mixture for test case 1.

w_r	9.245899051158928e-004
w_p	1.054389119543879e-003
C_{vr}	2.119630293487619e-003 kJ/g K
C_{vp}	7.3e-04 kJ/g K
Γ_r/v_r	2.65428833544628 g/cc
Γ_g/v_p	0.872503835298257 g/cc
C_v	1.460560661525277e-003 kJ/g K
Γ/v	2.03202871115568 g/cc
c_T	7.52575364595788 km/s
c_S	7.66179726700490 km/s

V.   DETAILS ON THE REACTANTS TEMPERATURE AND AN ALTERNATIVE FIX

To be more explicit, the temperature formulas used by [1] and their p-T equilibration "fixes" for imaginary temperature are explored next. Furthermore, a new "fix" is proposed which keeps the temperature as a continuous function of density and energy. The previous example case is then computed with the new fix.

The reactants temperature, equation (37) of [1], is given as:

$$T_r(\rho, e) = T_r^s(\rho) \left(\frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 \right)^{\frac{1}{1+\alpha_{st}}} \tag{40}$$

Note that the temperature along the reference isentrope, $T_r^s(\rho)$, is given by integrating the thermodynamic identity [4] [5]:

$$\Gamma(v) = -\frac{v}{T} \left(\frac{\partial T}{\partial v} \right)_s \tag{41}$$

or in terms of density:

$$\Gamma(\rho) = \frac{\rho}{T} \left(\frac{\partial T}{\partial \rho} \right)_s \tag{42}$$

With the Grüneisen parameter, for the Davis reactants EOS, as a piecewise function:

$$\Gamma_r(\rho) = \begin{cases} \Gamma_r^0, & \rho < \rho_0 \\ \\ \Gamma_r^0 + Zy, & \rho \geq \rho_0 \end{cases} \tag{43}$$

where $y = 1 - \rho_0/\rho$ and Z is a parameter. Then the temperature along the reference isentrope, $T_r^s(\rho)$, is given by:

$$T_r^s(\rho) = \begin{cases} T_0 \left(\frac{\rho_0}{\rho} \right)^{-\Gamma_r^0}, & \rho < \rho_0 \\ \\ T_0 \exp(-Zy) \left(\frac{\rho_0}{\rho} \right)^{(-\Gamma_r^0 + Z)}, & \rho \geq \rho_0 \end{cases} \tag{44}$$
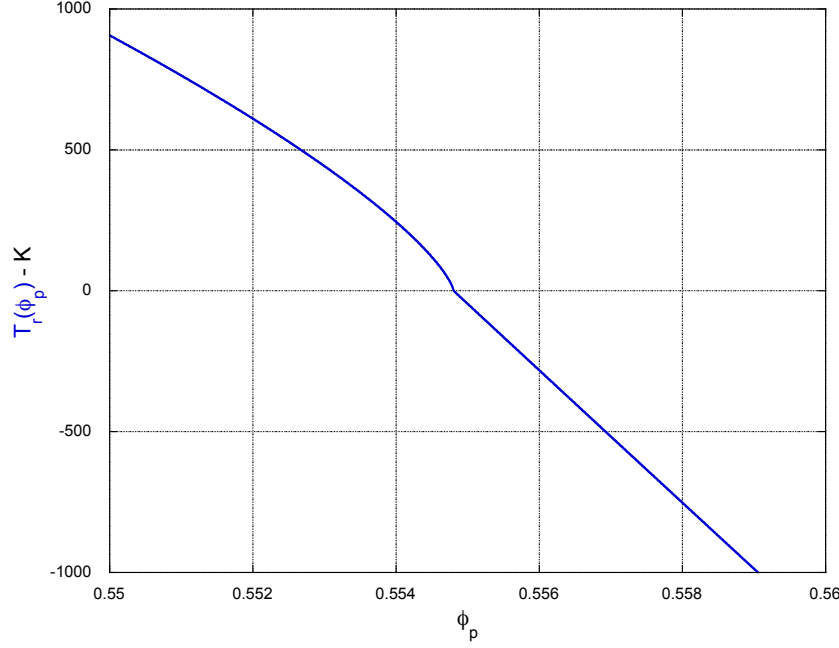
FIG. 4. $T_r(\phi_p)$ of the new model, equation (47), in the vicinity of where the new model switches from a variable specific heat to a constant specific heat model to avoid imaginary temperature values.

Clearly for equation (40), whenever the term:

$$\frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 \tag{45}$$

becomes negative, the temperature will become imaginary. This is of course problematic, as one might wander in into that region as a part of the root finding procedure. The authors of [1] proposed the following fix:

$$T_r(\rho, e) = \begin{cases} T_r^s(\rho) \left(\frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 \right)^{\frac{1}{1 + \alpha_{st}}}, & \frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 > 0 \\ \\ T_r^s(\rho) + \frac{e - e_r^s(\rho)}{C_{vr}^0}, & \text{otherwise} \end{cases} \tag{46}$$

The issue that arises with such a fix is that the temperatures are discontinuous when the switch happens, as seen in figure 3. Worse than that, it could potentially lead to multiple roots in $F(\phi_p)$, although that is not the case for the particular example shown in figure 2.

One simple fix, with a constant specific heat model, that maintains continuity of temperature could be:

$$T_r(\rho, e) = \begin{cases} T_r^s(\rho) \left(\frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 \right)^{\frac{1}{1 + \alpha_{st}}}, & \frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 > 0 \\ \\ T_r^s(\rho) \left(\frac{1 + \alpha_{st}}{C_{vr}^0 T_r^s(\rho)} \left[e - e_r^s(\rho) \right] + 1 \right), & \text{otherwise} \end{cases} \tag{47}$$

With this modified "fix," one has a continuous reactants temperature as a function of both ρ and e (and thus ϕ_p), while avoiding imaginary temperatures. See figure 4. Note that if one has a preexisting Newton method, one would have a different set of partial derivatives that will need to be appropriately modified for

this new fix. Note that the new function is C^0 continuous, so the derivatives will still be discontinuous, and although one could build in higher orders of continuity, there is little numerical benefit as the derivative is singular at $T_r = 0$.

VI. A SECOND TEST CASE, WHICH TESTS THE "EXPANSION" BRANCH OF THE REACTANTS

Here, a second test case is given, which explores the expansion branch of the reactants reference isentrope. Table 6 gives the density, specific internal energy and mass fraction of products for the second test case. Table 7 gives the resulting p-T equilibrium solution and Table 8 the thermodynamic states. Note that in this relatively low pressure, expanded case, the volume fraction of the products, ϕ_p, is substantially larger than the mass fraction of products, λ. This is commensurate with products density being substantially lower than the reactants density.

Table 6. Mixture density, mixture energy and mass fraction for the test case 2.

ρ	e	λ
0.5 g/cc	4 kJ/g	0.5

Table 7. p-T equilibrium for the test case 2.

ϕ_p	0.702467432347088
ρ_r	0.840244152000308 g/cc
ρ_p	0.355888384981352 g/cc
e_r	7.31714278655086 kJ/g
e_p	0.682857213449136 kJ/g
$p = p_r = p_p$	0.158795109201391 GPa
$T = T_r = T_p$	924.496190305791 K
c	0.790266 km/s

Table 8. Thermodynamic properties of reactants, products and equilibrium mixture for test case 2.

w_r	2.73651261423785e-002
w_p	7.18879123838186
C_{vr}	2.05555763736781e-003 kJ/g K
C_{vp}	7.3e-04 kJ/g K
Γ_r/v_r	0.704124599376258 g/cc
Γ_g/v_p	0.219398870062364 g/cc
C_v	1.43453777688757e-003 kJ/g K
Γ/v	0.115049271883312 g/cc
c_T	0.744521130389554 km/s
c_S	0.790271555577099 km/s

VII. A THIRD CASE WHERE THE NEW "FIX" IS NEEDED TO AVOID MULTIPLE ROOTS

If a slightly lower energy is taken in the previous tests case (see table 9) one can see that without the alternative fix of section IV, one has a multiplicity of pressure-temperature equilibration roots. See figure 5. Only one of them is consistent with the proper thermodynamic $T_r(\rho, e)$. See table 10 for the proper thermodynamic $p - T$ point and table 11 for the thermodynamic states. See Table 12 for the inconsistent root. Note that the alternative fix of equation (47) has only one root, which is the thermodynamically consistent root. Importantly, without a proper fix, both bisection-like and Newton-like methods for equation (46) may find nonphysical solutions.
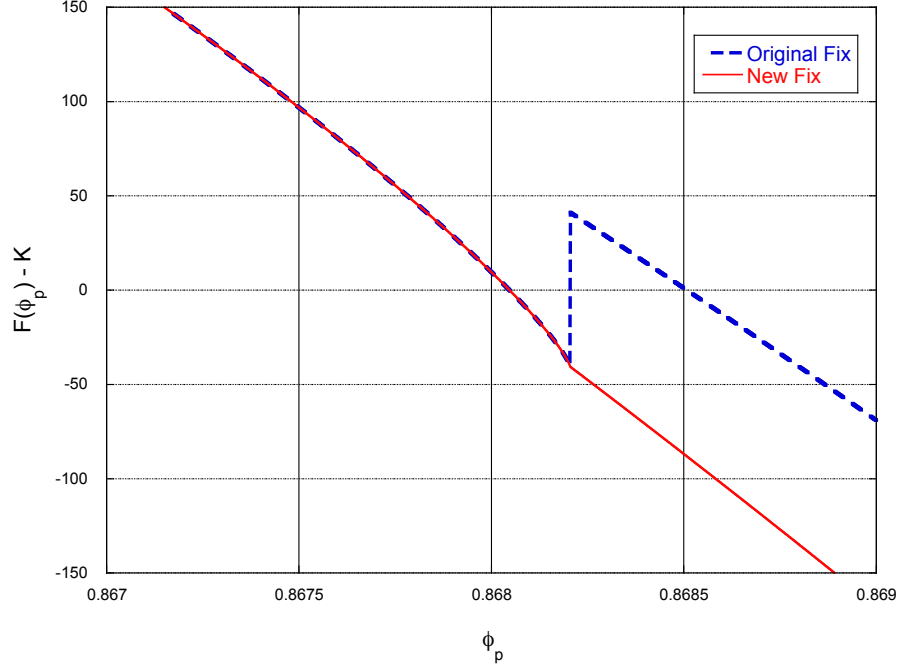
FIG. 5. Comparison of $F(\phi_p)$ of the new fix, equation (47), versus the original fix, equation (46), for case 3 where the old fix has two roots.

Table 9. Mixture density, mixture energy and mass fraction for the test case 3.

ρ	e	λ
0.5 g/cc	2.7 kJ/g	0.5

Table 10. p-T equilibrium for the test case 3.

ϕ_p	0.868047157111614
ρ_r	1.89461624719572 g/cc
ρ_p	0.288002786429096 g/cc
e_r	5.37597427519411 kJ/g
e_p	0.024025724805885 kJ/g
$p = p_r = p_p$	0.007549562431386 GPa
$T = T_r = T_p$	28.0070998667272 K
c	0.233496 km/s

Table 11. Thermodynamic properties of reactants, products and equilibrium mixture for test case 3.

w_r	1.96501661128695e-002
w_p	77.9749211775576
C_{vr}	4.45084206837434e-004 kJ/g K
C_{vp}	7.3e-04 kJ/g K
Γ_r/v_r	1.58768841515002 g/cc
Γ_g/v_p	0.178248778797248 g/cc
C_v	5.877249866662125e-004 kJ/g K
Γ/v	0.221645948173554 g/cc
c_T	0.226463287679891 km/s
c_S	0.233495675177352 km/s

Table 12. Thermodynamically inconsistent p-T equilibrium for test case 3.

ϕ_p	ρ_r	ρ_p	e_r	e_p	$p = p_r = p_p$	$T = T_r = T_p$	c
0.868508	1.90126 g/cc	0.287850 g/cc	5.34889 kJ/g	0.0511070 kJ/g	0.0123637 GPa	65.1146 K	0.258900 km/s

VIII. A FOURTH CASE, WHERE $F(\phi_p)$ IS NON-MONOTONIC

When one has a small amount of products, by mass, but in a highly expanded region, the function $F(\phi_p)$ can be non-monotonic. Furthermore, in such cases, even though the mass fraction of products, λ, may be small, the volume fraction of products, ϕ_p, may not. Table 13 is one such example. As can be seen in the table, there is very little, by mass, products for this case. But, by volume, the mixture is nearly 90% products by volume, see Table 14 and 15. Note that for such a case, the mixture sound speed is extremely low, less than 5 m/s. This is due to the relative ease of compressing the gas, but the relatively high density of the mixture. See figure 6 for the plot of $F(\phi_p)$, showing its non-monotonic behavior. And, even though there is only a single root, the vast majority of initial guesses for a Newton-like method would be quite problematic. Note the inset zoomed in for small values of ϕ_p.

Table 13. Mixture density, mixture energy and mass fraction for the test case 4.

ρ	e	λ
0.2 g/cc	5.7 kJ/g	10^{-4}

Table 14. p-T equilibrium for the test case 4.

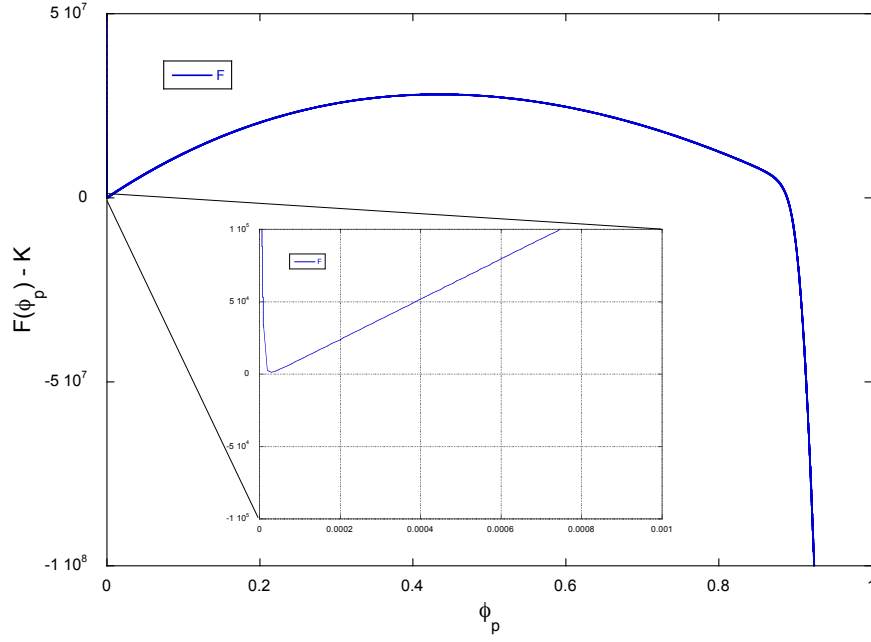|	
ϕ_p	0.889226996468719
ρ_r	1.80531351164031 g/cc
ρ_p	2.24914449059955e-005 g/cc
e_r	5.70054231654439 kJ/g
e_p	0.277376872685692 kJ/g
$p = p_r = p_p$	3.87723164746165e-6 GPa
$T = T_r = T_p$	379.968318783949 K
c	4.67091e-3 km/s

FIG. 6. $F(\phi_p)$ for the non-monotonic example of test case 4.

Table 15. Thermodynamic properties of reactants, products and equilibrium mixture for test case 4.

w_r	5.77911163431921e-002
w_p	1146729.26115069
C_{vr}	1.17379118549171e-003 kJ/g K
C_{vp}	7.3e-04 kJ/g K
Γ_r/v_r	1.51285272275457 g/cc
Γ_g/v_p	1.39782080946271e-005 g/cc
C_v	1.24299021652142e-003 kJ/g K
Γ/v	8.28130742189879e-006 g/cc
c_T	4.66916849103467e-003 km/s
c_S	4.66925520306313e-003 km/s

IX. OBTAINING EQUILIBRATION, WHEN PROVIDING PRESSURE AND DENSITY

During initialization and at boundary conditions, specification of pressure and density is often the natural choice. In such circumstances, we clearly can specify $p = p_r = p_p$, but still need to determine the mixture energy under the assumption of $T_r = T_p$. A similar strategy is employed to reduce the the system of equations to a single nonlinear root finding problem. But, here, we are given the mixture density, ρ, and mass fraction of products, λ and the mixture pressure, p. Now, the mixture energy, e, is the unknown. The formulation is still constructed in terms of the volume fraction of products, ϕ_p. As such, the densities of the reactant and

products are given as before:

$$\rho_r = \frac{\rho}{1-\phi_p}(1-\lambda) \text{ and } \rho_p = \frac{\rho}{\phi_p}\lambda. \tag{48}$$

With these and the Mie–Grüneisen EOSs, equations (17-18), now written in terms of $e(\rho, p)$:

$$e_r\left(\rho_r, p_r\right) = e_r^s(\rho_r) + \frac{p_r - p_r^s(\rho_r)}{\rho_r \Gamma_r(\rho_r)} \tag{49}$$

and

$$e_p\left(\rho_p, p_p\right) = e_p^s(\rho_p) + \frac{p_p - p_p^s(\rho_p)}{\rho_p \Gamma_p(\rho_p)}, \tag{50}$$

we can construct the difference in temperature, as was done previously, and look for the root of the equation:

$$F_e(\phi_p) = T_r\left(\rho_r(\rho, \lambda, \phi_p), e_r(\rho_r, p_r)\right) - T_p\left(\rho_p(\rho, \lambda, \phi_p), e_p(\rho_p, p_p)\right) = 0. \tag{51}$$

Again, this is really the same function as previously, namely the difference in temperatures, but the information going into constructing the function is different, thus the subscript e in the F_e to note that e is the unknown now, instead of pressure.

X. ROOT FINDING PROCEDURE

Here, a set of techniques are constructed to robustly find the solution to the $p - T$ equilibrium state. The technique is the same for determining $p(\rho, e, \lambda)$ as it is for $e(\rho, p, \lambda)$, although separate functions/subroutines will be needed for each specific case. Here, we will just use $F(\phi_p)$ generically. The essential algorithm, that is both relatively fast and more importantly quite robust is a combination of modified versions of the well known algorithms: Secant method and Bisection method. Furthermore, if incorporated into a hydrodynamic algorithm, keeping track of ϕ_p for each cell will yield a good starting guess for the numerical root finding procedures. As shown in figure 1, the function $F(\phi_p)$, will become singular at $\phi_p = 0$ or $\phi_p = 1$, due to the density singularity of equations (14-15), if λ is not also 0 or 1. Clearly, there is no physical meaning to ϕ_p either less than zero or greater than one. This sets a clear bound on ϕ, and for physical parameters F will tend toward infinity as ϕ_p tends toward zero and F will tend towards negative infinity as ϕ_p tends towards unity. For well-posed EOSs, there should only be a single value of ϕ_p that satisfies the equilibrium conditions. This unique solution should correspond to maximizing the entropy or minimizing the free energy of the system [4]; again, this presumes well-posedness of both the reactants and products EOSs over all thermodynamically relevant EOS space [8].

Prior to elucidating the details of the root finding procedure, there should be limits on how close λ is to 0 or 1 so as to have a meaningful equilibration, which gets into details of computer precision. Here, it is presumed that double precision is being utilized, which generally utilizes a 52 bit significand, which yields $\approx$16 significant figures for double precision numbers. There is not much point in performing $p - T$ equilibration when λ is sufficiently close to 0 or 1. We have chosen, somewhat arbitrarily, to presume the EOS is simply just reactants when $\lambda < 10^{-14}$ and completely products when $\lambda > 1 - 10^{-14}$. These limits are significantly closer to the bounds than is generally done in typical hydrocode $p - T$ equilibration procedures, and can be modified as seen fit. Keep in mind, the CJ state of detonation is quite sensitive to having these cutoff values too far away from $\lambda = 1$, as some thermodynamic values scale like $\sqrt{1-\lambda}$. Also, for material that is initially all reactants, i.e. $\lambda = 0$, of course $\phi_p = 0$ as well. But, if one has a tiny bit of chemistry to raise $\lambda > 10^{-14}$ during a time step, the previous value of $\phi_p = 1$ will lead to singular behavior. It is worth taking $\phi_p = \max(\phi_p, \frac{1}{2}\lambda)$, which avoids the singularity.

We begin the procedure with a single initial guess of ϕ_p. Here, only one initial guess is provided, say from the hydrocode, subject to the previous limitation on λ. If one is initializing for the first time, and there is no

previous hydrocode solution to use, one can simply chooses $\phi_p = \lambda$, which is equivalent to presuming equal densities between reactant and products. The Secant method [9] needs 2 initial guesses to begin iteration. A second value of ϕ_p should be a small perturbation from the starting guess. The smallness of the perturbation is to ensure that if one is already close to the root, a small perturbation will not require many additional steps to reach convergence. One must be careful in deciding how small is small enough, and not too small. Also, one must be careful when ϕ_p is near the limits of 0 and 1, so that the the perturbation does not exceed those limits. Keep in mind that long reaction tails can lead to λ and ϕ_p values extremely close to 1, and numerical diffusion, say upstream of a captured shock/detonation wave can lead to values extremely close to 0. It is desirable to build in those limits to maintain robustness of the algorithm. Here, a perturbation of ϕ_p is chosen to be:

$$\delta\phi_p = \min\left(\frac{1}{10}\left|1 - \phi_p\right|, \frac{1}{10}\phi_p, 10^{-8}\right) \tag{52}$$

Under normal circumstances, 10^{-8} is chosen, unless ϕ_p is sufficiently close to its bounds of 0 or 1, in which case one of the first 2 choices in the min function are activated. So, with a starting guess of ϕ_p^1, we can take the second value to be:

$$\phi_p^2 = \begin{cases} \phi_p^1 + \delta\phi_p, & \phi_p^1 < \frac{1}{2} \\ \\ \phi_p^1 - \delta\phi_p, & \text{otherwise} \end{cases} \tag{53}$$

The $\pm$ choice above is simply to take the perturbation further away from the bounds of 0 or 1. With these 2 values, and the $F(\phi_p^1)$ and $F(\phi_p^2)$, we can use the Secant method to determine an improved trial guess value for $\hat{\phi}_p^3$ as:

$$\hat{\phi}_p^3 = \phi_p^2 - F(\phi_p^2)\frac{\phi_p^2 - \phi_p^1}{F(\phi_p^2) - F(\phi_p^1)} \tag{54}$$

To ensure this new, supposedly improved, value of ϕ_p doesn't exceed the physical bounds of $0 < \phi_p < 1$, we take the actual next value to be:

$$\phi_p^3 = \begin{cases} \hat{\phi}_p^3, & \text{if } 0 < \hat{\phi}_p^3 < 1 \\ \\ \frac{\max(\phi_p^1, \phi_p^2) + 1}{2}, & \text{if } \hat{\phi}_p^3 \geq 1 \\ \\ \frac{\min(\phi_p^1, \phi_p^2)}{2}, & \text{if } \hat{\phi}_p^3 \leq 0 \end{cases} \tag{55}$$

The last two cases of the above essentially march halfway towards to bounds of ϕ_p, if $\hat{\phi}_p^3$ is outside the bounds. Under most circumstances, the first case, $\phi_p^3 = \hat{\phi}_p^3$ is chosen, which is the standard Secant method. This procedure is repeated until one of 3 stopping criteria are met. These are:

1) Number of iterations has reached 20

2) If $F(\phi_p^n) < \text{tol}$

3) If $|\phi_p^n - \phi_p^{n-1}| < \Delta\phi_{min}$.

Here, a near machine precision limit of $\Delta\phi_{min} = 10^{-14}$ is chosen. A very small value of tol $= 10^{-10}$K is chosen. Recall F has dimensions of temperature, and since typical values of T will be O(1000 K), this represents a very tight, near machine precision, tolerance as well.

If the number of Secant iterations is exceeded, then a modified Bisection method is employed. For most cases, with a good initial guess, the Bisection method will not be needed, as convergence is often obtained

with 1-5 iterations. An example of where Secant and Newton-like schemes fail is when F is non-monotonic, and a poor initial guess is chosen, such as in test case 4. Recall that the standard Bisection method [9] needs a bracketed set of initial ϕ_p values. Even though we know $\phi_p = 0$ and $\phi_p = 1$ bracket the root, taking both limits would lead to generation of NaNs. But, if we know those are limiting cases, and we know the sign of F is positive for ϕ_p small enough and negative for ϕ_p large enough, one can start at $\phi_p = 1/2$, evaluate the sign of $F(1/2)$, and if its positive, increase ϕ_p by $1/4$, if negative, then decrease by $1/4$. Continue repeating this procedure of increasing/decreasing ϕ_p by increments of $(1/2)^n$, based on the sign of $F(\phi_p)$, for 52 iterations, and double precision will be reached.

Once ϕ_p has been determined, the thermodynamic states, p and T can be evaluated. The sound speed, c, can be evaluated either via thermodynamic identities [4] or by finite differences of equation (39). Note that the partial derivatives in equation (39) are held at fixed e or fixed ρ, which means that ϕ_p is not fixed, and that implies that each of the finite difference points needs to perform a full $p - T$ equilibration. That sounds like a lot of additional computation, but for small changes to e and ρ, the $p - T$ equilibrium values of ϕ_p change very little. So, very few iterations are needed at each of the finite difference points. Here, we've chosen relative perturbations of 10^{-7} for e and ρ and second order central differences about the equilibrium point. This appears to yield approximately 10 significant figures in the sound speed computation. It is likely that direct thermodynamic computation of the sound speed will both be faster and more accurate.

XI.   APPENDIX - THERMODYNAMIC PROPERTIES OF THE EQUILIBRIUM MIXTURE

In the present section, the thermodynamic properties, i.e. sound speed, specific heat etc. of the partially reacted equilibrium mixture are described. A detailed description of the current approach to compute the thermodynamic properties is provided in [4].

Following the root finding procedure for $p-T$ equilibrium, the isothermal sound speed, c_T for the equilibrium mixture is calculated as weighted average of the individual reaction component values:

$$\frac{1}{(\rho c_T)^2} = w_r + w_p \tag{56}$$

where, $w_i = \frac{\lambda_i}{(\rho_i c_{T_i})^2}$ and $c_{T_i}^2 = \left(\frac{\partial p_i}{\partial \rho_i}\right)_{T_i}$, the expressions for the reactants and products isothermal sound speed, c_{T_i} are presented in the next sub-sections.

Using the weights ($w_i^{'s}$), the isochoric specific heat and Grüeneisen co-efficient for the reaction mixture are computed as:

$$C_v = \lambda_r C_{vr} + \lambda_p C_{vp} + \frac{w_r w_p}{w_r + w_p}\left[C_{vr}\frac{\Gamma_r}{v_r} - C_{vp}\frac{\Gamma_p}{v_p}\right]^2 T \tag{57}$$

$$\frac{\Gamma}{v} = \frac{w_r C_{vr}\frac{\Gamma_r}{vr} + w_p C_{vp}\frac{\Gamma_p}{vp}}{(w_r + w_p)C_v} \tag{58}$$

Next, using equations (56)-(58) the isentropic sound speed for the equilibrium mixture is calculated:

$$(\rho c_S)^2 = (\rho c_T)^2 + \left(\frac{\Gamma}{v}\right)^2 C_v T \tag{59}$$

The isothermal sound speed for the reaction mixture given by equation (56) is calculated using the weights, $w_i^{'s}$ for reactants and products. To compute $w_i^{'s}$, the isothermal sound speed for the indivuidual reaction

components is calculated. In this section, the details to derive the isothermal sound speed from Davis reactants EoS are presented.

The Davis reactants EoS form in terms of $p_r(\rho, T)$ [10] is expressed as:

$$p_r(\rho, T) = p_r^s(\rho) + \frac{\rho \Gamma_r(\rho) C_{vr}^0 T_r^s(\rho)}{1 + \alpha_{st}} \left[\left(\frac{T}{T_r^s(\rho)} \right)^{1+\alpha_{st}} - 1 \right] \tag{60}$$

Using equation (60), the isothermal sound speed for reactants is calculated as:

$$c_{T_r}^2 = \left(\frac{\partial p_r}{\partial \rho} \right)_T = \frac{dp_r^s(\rho)}{d\rho} + \frac{C_{vr}^0}{1 + \alpha_{st}} \left[T_r^s \left\{ \Gamma_r + \rho \frac{d\Gamma_r}{d\rho} \right\} \left\{ \left(\frac{T_r}{T_r^s} \right)^{1+\alpha_{st}} - 1 \right\} - \rho \Gamma_r \frac{dT_r^s}{d\rho} \left\{ \alpha_{st} \left(\frac{T_r}{T_r^s} \right)^{1+\alpha_{st}} + 1 \right\} \right] \tag{61}$$

where, the derivative of $p_r^s(\rho)$, $\Gamma_r(\rho)$ and $T_r^s(\rho)$ with respect to ρ is obtained as:

$$\frac{dp_r^s(\rho)}{d\rho} = \begin{cases} \frac{\hat{p}\rho_0}{\rho^2} \left[4B exp(4By) \right], & \rho < \rho_0 \\[3mm] \frac{\hat{p}\rho_0}{\rho^2} \left[\sum_{j=1}^3 \frac{(4B)^j y^{j-1}}{(j-1)!} + C \frac{(4B)^4 y^3}{3!} - \frac{2y(y+1)}{(y-1)^5} \right], & \rho \geq \rho_0 \end{cases} \tag{62}$$

$$\frac{d\Gamma_r(\rho)}{d\rho} = \begin{cases} 0, & \rho < \rho_0 \\[3mm] -\frac{Z}{\rho_0}, & \rho \geq \rho_0 \end{cases} \tag{63}$$

$$\frac{dT_r^s(\rho)}{d\rho} = \begin{cases} \frac{T_0 \Gamma_r^0}{\rho_0} \left(\frac{\rho}{\rho_0} \right)^{\Gamma_r^0 - 1}, & \rho < \rho_0 \\[3mm] \frac{T_0}{\rho_0} exp(-Zy) \left(\frac{\rho}{\rho_0} \right)^{\Gamma_r^0 + Z - 1} \left[\Gamma_r^0 + Z \left(1 + \frac{\rho}{\rho_0} \right) \right], & \rho \geq \rho_0 \end{cases} \tag{64}$$

The Davis products EoS expressed in terms of $p_p(v, T)$ [1] as:

$$p_p(v, T) = p_p^s(v) + \frac{\Gamma_p C_{vp}}{v} [T - T_p^s(v)] \tag{65}$$

The isothermal sound speed for the products is calculated using the EoS definition equation (65):

$$c_{T_p}^2 = \left(\frac{\partial p_p}{\partial \rho} \right)_T = -\frac{1}{\rho^2} \left(\frac{\partial p_p}{\partial v} \right)_T \tag{66}$$

where,

$$\left(\frac{\partial p_p}{\partial v} \right)_T = \frac{dp_p^s(v)}{dv} + \left[\frac{C_v}{v} \frac{d\Gamma_p}{dv} - \frac{\Gamma_p C_v}{v^2} \right] [T - T_p^s(v)] - \frac{\Gamma_p C_v}{v} \frac{dT_p^s(v)}{dv} \tag{67}$$

The derivative of $p_p^s(v)$, $\Gamma(v)$ and $T_r^s(v)$ with respect to v is calculated as:

$$\frac{dp_p^s(v)}{dv} = -p_c \frac{[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}]^{a/n}[4a^2 + k(k-1)(1 + (v/v_c)^{2n})^2 + 2a(2k - 1 + (2k + 2n - 1)(v/v_c)^{2n})]}{(v/v_c)^{k+a} v(k - 1 + a)[1 + (v/v_c)^{2n}]^2} \tag{68}$$

$$\frac{d\Gamma_p(v)}{dv} = -\frac{4an(1-b)(v/v_c)^{2n}}{v[1+(v/v_c)^{2n}]^2} \tag{69}$$

$$\frac{dT_p^s(v)}{dv} = -T_c(v/v_c)^{-k-a(1-b)}\frac{\left[\frac{1}{2}(v/v_c)^n + \frac{1}{2}(v/v_c)^{-n}\right]^{a(1-b)/n}[(k-1)(v/v_c)^{2n} + k - 2ab + 2a - 1]}{v_c[1+(v/v_c)^{2n}]} \tag{70}$$

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